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Mesoscale Science at Extreme Conditions Workshop

a Momentum Initiative Workshop

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August 5-8, 2019

at Los Alamos National Laboratory and La Posada de Santa Fe, Santa Fe, NM

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1. Introduction

1.1 Executive Summary

In early August 2018, experts in both modeling approaches and experimental techniques active at the mesoscale gathered in Los Alamos and Santa Fe, New Mexico to discuss the current state-of-the-art for modeling, simulation, and experiments available at the mesoscale, information that can be used to inform and/or validate both mesoscale and larger-length scale models, and opportunities for future work and collaboration. The overarching goal was to identify needs within LANL's community that mesoscale science (models or experiments) could address. In addition, the workshop intended to identify gaps that exist within this field that could inform future research directions and the formation of advantageous collaborative efforts.

This document and its addendum are meant to constitute a summary of topics and issues that were discussed during this workshop. The workshop consisted of technical talks from both academic and LANL scientists that covered a wide range of topics including: Metals, High Explosives, Surface Science, and Manufacturing. The technical topics from each session are summarized, with specific technical presentations highlighted to illustrate state-of-the-art techniques and capabilities available in the field now. Current and future collaboration opportunities are discussed for each topical area that was included in the workshop. This document also includes recommendations and conclusions determined from these technical presentations and other discussions that took place during the workshop. Finally, speaker abstracts and the final agenda are included at the end of this document.

At the end of the workshop it was clear that there have been significant advancements within the field. A major need identified at LANL was the need for microstructurally aware material models, which already exist in the greater scientific community for common industrial materials and applications. LANL is particularly interested in very complex materials (arguably the most complex materials) under extreme conditions (high pressure, temperature, and strain rate regimes), and complicated multi-physics processes. Integrating several physical processes into microstructurally aware material models remains a challenge within the community. While there is some work addressing more challenging material classes (for example, multiple principal element alloys), there is still a need for further model development and additional experiments studying the connected and complex deformation processes that control the overall material response.

Consequently, many mesoscale modeling approaches only account for the dominant deformation mechanisms and physical processes for a specific application. This requires conclusive evidence of what the dominant deformation mechanisms and physical processes are for an application. This information is typically provided by experiments, however in experimental work is it extremely difficult to decouple the active mechanisms and processes to determine which has the dominant effect on the overall material response. Hence, there are still many remaining questions about what are the dominant physics active during key processes, how multiple physics processes couple and interact, and how this interplay corresponds to observed macro-scale material response.

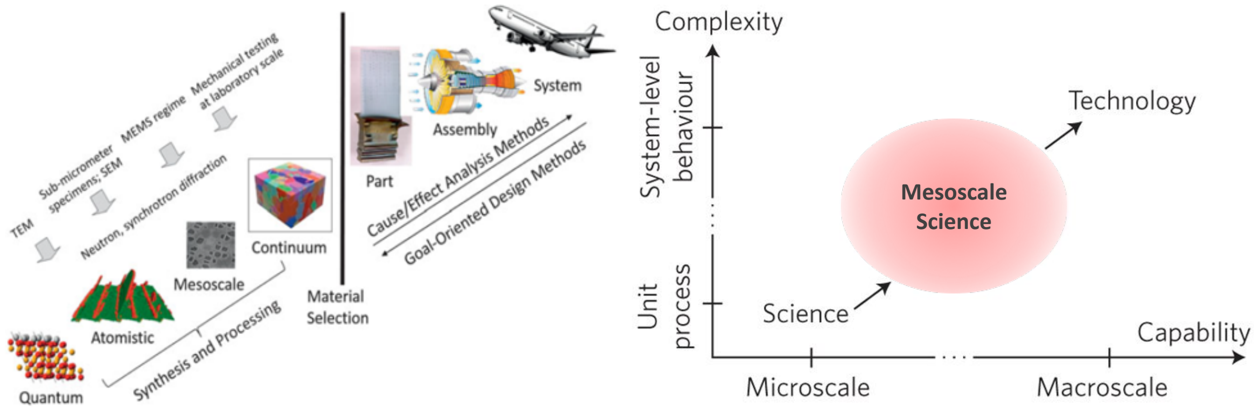

Figure 1: Diagrams showing the role of mesoscale science in comparison to other micro- and macro-scale techniques. (D. L. McDowell and R. A. LeSar MRS Bulletin 41 (8) 587-593 (2016); S. Yip and M. Short, Nat. Mater. (12) 774-777 (2013)).

1.2 Background

The dynamic thermomechanical responses of materials under extreme loading environments are often dominated by the interactions of defects and interfaces. For example, polymer-bonded explosives might be initiated under weak shock impacts that would be insufficient to drive a reaction if the material response were homogeneous. Within metals, a prescribed deformation associated with a shock wave may be accommodated by crystallographic slip, void nucleation and growth, and fracture; the competition amongst these processes is often influenced by the behavior of grain boundaries. In the case of corrosive environments, surface pits often act as sites for crack initiation. These cracks then tend to propagate along grain boundaries within the material, moving along both the surface of the sample and also down into the bulk material. Furthermore, modifications to the manufacturing processes to make these materials often modifies the details of such defect and interface structures in a manner that is not obvious at the outset and can have profound effect of the macroscale performance of the material *in-situ*. Direct numerical simulation at the mesoscale offers insight into these physical processes that can be invaluable to the development of macroscale constitutive theories. However, this approach requires that the mesoscale models adequately represent the nonlinear thermomechanical response of individual constituents, properly accounting for the details of such defects and their collective interactions.

The purpose of this workshop is to provide a platform for researchers working on state-of-the-art mesoscale science, including both modeling and experimental efforts, to meet and discuss the investigation of complex material systems. A particular interest of the workshop is how mesoscale science can help to elucidate the material deformation processes that occur when materials are subject to extreme environmental and loading conditions relevant to furthering the LANL national security mission. This includes, but is not limited, to shock loading, extreme

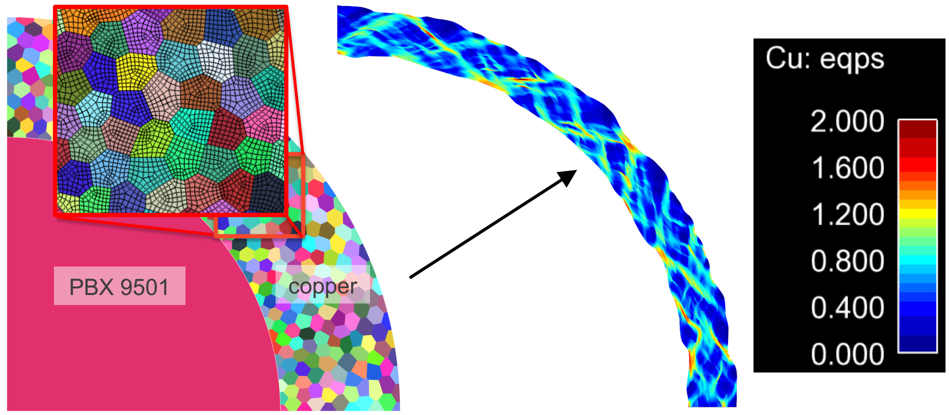

Figure 2: Mesoscale simulation of the explosively driven expansion of a polycrystalline cylindrical shell using the LANL hydrocode, FLAG. The grain structure is explicitly resolved and each grain is modeled using a single crystal model for copper. Contour plot at right shows the magnitude of plastic strain concentrated into shear bands, which lead to the formation of fragments.

temperature and pressure environments, corrosive environments, and radiation environments. Figures 2 and 3 highlight some aspects of ongoing work at LANL in this area. For example, Figure 2 depicts recent simulations from ASC-PEM in which the microstructure of polycrystalline copper gives rise to heterogeneous deformation fields providing a mechanism for localization of deformation and, ultimately, the formation of distribution of fragments. Figure 3 illustrates the heterogeneity in plastic strain and temperature fields of an idealized PBX microstructure from a modeling strategy developed in the LANL LDRD-DR project led by Kyle Ramos and Marc Cawkwell.

With such efforts underway, one objective of the workshop was to identify where we are leading, where we are lagging, and what opportunities for collaboration might further our interests in this area of research. The workshop welcomed talks and discussion on mesoscale modeling approaches, particularly those who have addressed issues of homogenization and scale-bridging, and those that have made the meso-to-macro link. Discussions on experimental work were also welcomed, particularly techniques that are mesoscale aware, can resolve microstructure and grain-level material behaviors, and non-destructive techniques operative at the mesoscale.

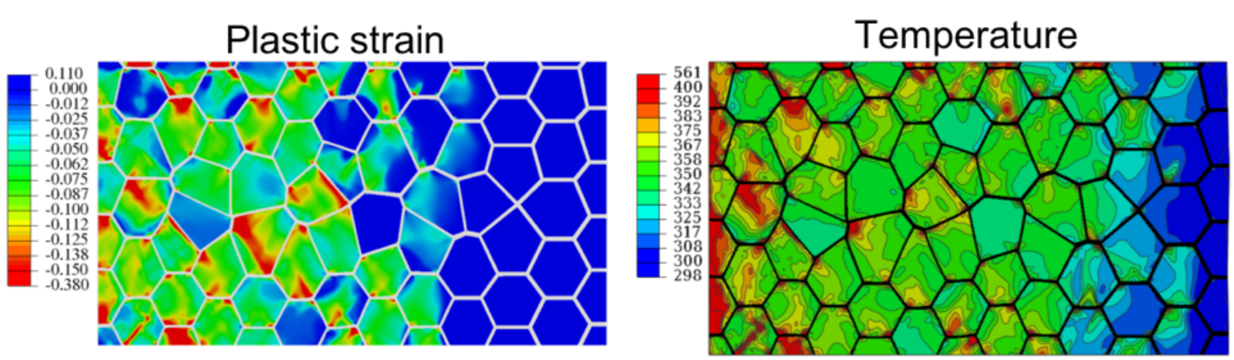

Figure 3: Mesoscale simulation of weak impact in Estane/RDX composite. Heterogenous plastic deformation leads to spatial variations in the temperature field.

2. Summary of Workshop Activities

Figure 4: Figure showing the balance needed between mission operations, science technology and engineering, and community relations (figure courtesy of John Sarrao).

The Mesoscale Science at Extreme Conditions Workshop took place on August 5-8, 2019, lasting four days. The first day (Monday August 5, 2019) at Los Alamos National Laboratory, featured presentations from LANL scientists. The remaining three days (August 6-8, 2019) took place at La Posada de Santa Fe, in Santa Fe. This part of the workshop was primarily focused on engaging with the academic community, both to gain an understanding of what is the state-of-the-art in modeling and experimental techniques and to foster new and current collaborations in the area of mesoscale science. Presentations were all 30 minutes to allow for questions and discussion. In addition, multiple breaks (also 30 minutes) and extended lunch periods were given to allow for offline discussion and interaction. A poster session was also held on Tuesday (August 6) evening. This allowed an additional opportunity for LANL scientists to present their work and meet with academics. Overall the workshop was well attended with 85 registrants in total.

Both Monday and Tuesday, John Sarrao (LANL, DDSTE) gave an opening talk "*Dynamic Mesoscale Materials Opportunities and Challenges*". In these talks, Dr. Sarrao discussed the Dynamic Mesoscale Materials Science Capability (DMMSC), which is meant to address a national scientific need for understanding performance and production at the mesoscale. In some ways this capability defines the need, and facilities such as The Matter-Radiation Interactions in Extremes (MaRIE) Facility is an example of a plausible solution that meets this need. In addition, the key elements of integration and balance were also discussed. An ultimate goal of DMMSC is the integration of material structure and processing to achieve desired material properties and performance. This should also support production science creating a balance between operations and mission, as shown in Figure 4.

Perhaps more focused on mesoscale science, Dr. Sarrao highlighted that DMMSC would fill a critical gap existing in time/length scales, which in turn would fill a knowledge gap present at the mesoscale. MaRIE in particular is intended to fill a capability gap by enabling resolutions between those addressed by DARHT and U1a facilities such as NIF and Z (see Figure 5). Some specific areas of interest were mentioned, including the performance of additively manufactured (AM) structural components, performance and safety of high explosives, and void collapse in energetic

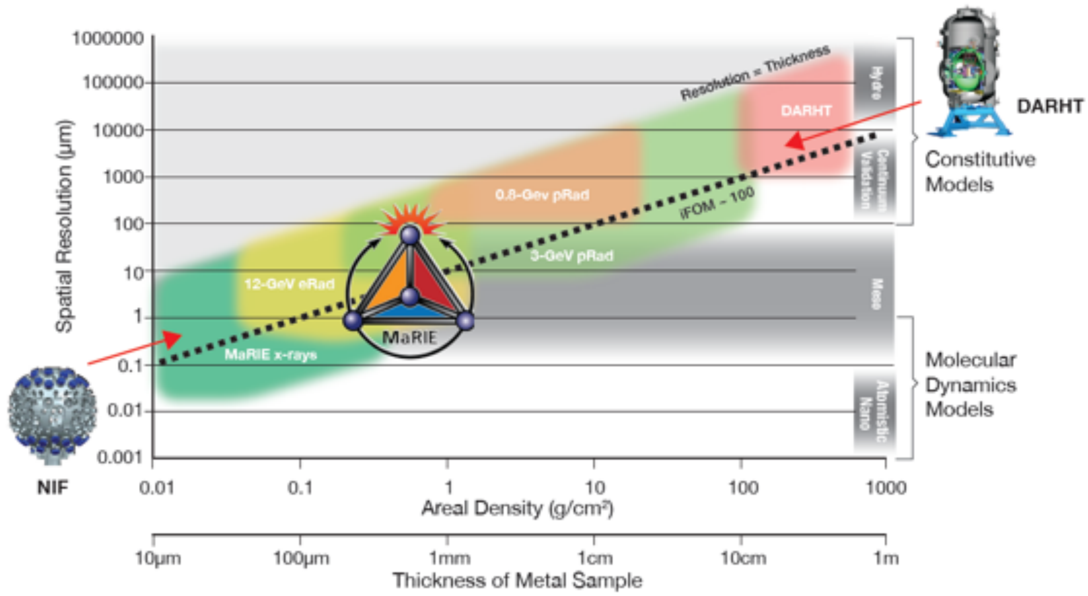

Figure 5: Diagram showing the gap in resolution that MaRIE aims to fill (figure courtesy of John Sarrao).

materials. All of these topics (and others) were addressed during this workshop. Overall, DMMSC promises to enable the rapid and confident deployment of new concepts, which will in turn allow for more cost-effective and scientifically rigorous approaches to be employed quickly and through-out the Laboratory.

The next sections summarize and discuss the topics covered in the workshop. More specifically, the sessions covered on Tuesday through Thursday of the workshop, broadly organized into the topical areas of Metals, High Explosives (HE), Surface Science, and Manufacturing, are summarized. These summaries include information about the current state-of-the-art, and takeaways about how far modeling and experimental techniques have evolved. Current and future collaborations are also discussed for each topic. Details of the talks and topics covered during the first day of the workshop (Monday) are included in the addendum to this report.

2.1 Metals

The Metals session took place on Tuesday August 6, 2019. This session was the only one to be broken up into symposia: Defective Metals, Multiple Principal Element/High Entropy Alloys, and Phase Transformations.

The Defective Metals symposium specifically focused on damaged or impure materials (i.e, metals with voids, cracks, impurities, inclusions, boundaries, etc.), and the subsequent impact of these imperfections on the overall material response. Speakers in this symposium included: Justin Wilkerson (Texas A&M University), Michael Short (Massachusetts Institute of Technology), and Giacomo Po (University of Miami).

Throughout the workshop, the fact that microstructure matters was heavily discussed by many, and this is a common thread across sessions. Dr. Wilkerson, who gave the first talk of this session, highlighted what modeling capabilities can do to address this problem now. He presented a dislocation-based crystal plasticity model for addressing damage in ductile materials undergoing high strain-rate loading conditions. In order to capture spall failure in ductile metals, void nucleation and growth must be accurately accounted for. It has been shown that voids nucleate and grow along material interfaces such as grain boundaries, hence grains and their boundaries must be accounted for in the model. Recent progress by this research group has demonstrated that relatively simple assumptions regarding the nature of grain boundaries in the damage process can represent many trends observed in experiment.

The Multiple Principal Element/High Entropy Alloys (MPEAs/HEAs) symposium targeted modeling and experimental technique that could address to overall material response of equimolar alloys with three or more components. Speakers in this symposium included: C. Cem Tasan (Massachusetts Institute of Technology), Irene Beyerlein (University of California, Santa Barbara), Amy Clarke (Colorado School of Mines), and Rajiv Mishra (University of North Texas).

The MPEAs/HEAs are massively alloyed systems. The talks in this symposium made it clear that the many components present in these systems have the potential to result in material properties that are a notable improvement over conventional binary alloys. However, also because there are so many components the parameter space that must be explored in order to identify optimal material properties is vast. This remains a standing challenge in both the modeling and experimental communities studying these materials. Furthermore, the unique composition of these materials also results in trends and deformation mechanisms that do not follow our traditional understanding of structural metals. For example, Dr. Clarke pointed out that the highest entropy system does not always correspond to the 'best' properties as one might think. Additionally, Dr. Mishra presented work that showed that deformation in hexagonal closed-packed (hcp) HEAs can change with the HEA composition and its processing, resulting in differences not seen in conventional hcp metals. While there is much work remaining to both understand and optimize these materials, they have the potential to offer LANL superior material properties under extreme loading conditions. MPEAs/HEAs systems are a potential example of a new concept that could have large impact at the DOE Laboratories if they could be employed in a cost-effective and rigorous approach. Such a process is a primary goal of DMMSC as described in Dr. Sarrao's presentations.

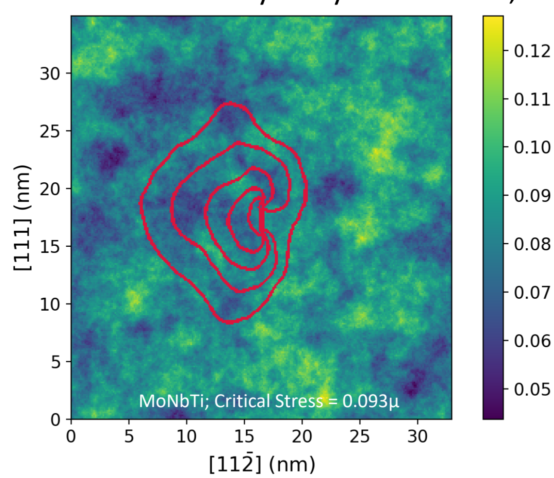

Figure 6: Phase field calculation of a dislocation loop expanding from Frank-Read source over time in MoNbTi MPEA. The colored surface shows the energy variation due to varying chemical composition in the alloy (figure courtesy of Irene Beyerlein).

The final symposium of the day was Phase Transformations, which focused on modeling and experimental work studying the kinetics of phase transformations, particularly under high-rate loading conditions. Speakers in this symposium included: Steve Niezgoda (Ohio State University), Ashley Bucsek (University of Michigan), and Matthew Freeman (LANL, P-23). Of particular interest to LANL are experimental techniques such as the work presented by Dr. Bucsek (see Figure 7). She presented recent work on 3D X-ray microscopy, an *in situ* technique that can provide sub-surface 3D information about voids, inclusions, cracks, and other heterogeneities. This technique is non-destructive and can be used on bulk samples, which allows for the possibility of a sample being studied repeatedly (for example after a load is applied). Crack initiation and propagation, and solidification are two examples of materials phenomena that can be studied with this approach. The method can be coupled with both near-field or far-field high energy diffraction microscopy (HEDM), which provides measurements at different resolutions (spanning 3-4 magnitudes in length scale) and correspondingly different measurements. For example, far-field HEDM can provide averaged grain orientation information, (elastic) strain tensor measurements, and phase contents. Near-field HEDM measurements, for example, can provide more detailed information about the actual grain structure (in contrast to the averaged values from far-field HEDM).

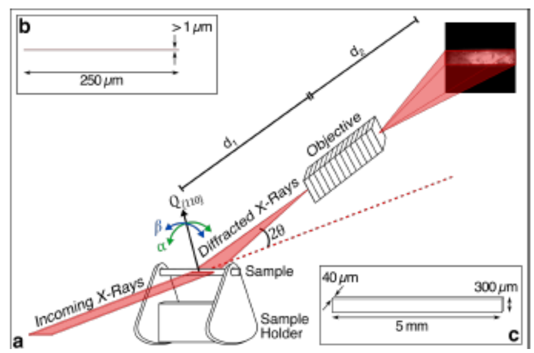

Figure 7: Schematic diagram of the dark-field X-ray microscopy technique. (A. Bucsek et al. Acta. Mater. (2019)).

Such an approach could study issues of crack and phase nucleation, and phase transformation kinetics, topics that are of great interest to LANL. Accurately modeling nucleation processes (for cracks or phase transformations) remains a premier challenge, and is highly dependent on microstructure. This type of approach could provide information about where in the grain structure and under what conditions nucleation occurs. This information is needed for the development of microstructurally aware material strength and damage models. Furthermore, it could provide statistical information about how crack networks grow and evolve. Such information could go to inform current fracture models implemented within the ASC code base (this work was highlighted in a poster and described later in Section 2.5). Finally, if this method evolves to be able to provide information such as the rate of phase growth, it could directly inform equation of state and other kinetics models.

Current and Future Collaboration Opportunities

Several of the speakers in this session have active collaborations with LANL staff. In fact, several speakers (Dr. Beyerlein, Dr. Clarke, and Dr. Niezogda) are former LANL employees. These faculty members have continued LANL collaborations that were initiated while they worked at LANL. For example, Abigail Hunter (LANL, XCP-5) has mentored multiple students from Dr. Beyerlein's group over several summers in the recent past. In addition to this, Dr. Wilkerson has a continuing collaboration with D.J. Luscher (LANL, T-3) from funding through ASC-PEM. Such collaborations are not only advantageous from a scientific perspective, but also for recruitment. For example, a new postdoc from Dr. Wilkerson's group is starting this year with Dr. Luscher.

Of course, there are still opportunities to build new collaborations. For example, Dr. Bucsek is a new faculty member at University of Michigan. Hence, she is likely looking to build new collaborations, and offers LANL a unique experimental technique. In an addition, it may be advantageous to build new collaborations with researchers working on MPEAs/HEAs, as these materials are relatively new to LANL and could offer desired material properties. In addition to the unique properties of the materials themselves, the methodologies and techniques developed for designing and optimizing material properties that produce *customized* material performance (materials with desired properties) is well aligned with LANL's PSPP goals (process, structure, properties, performance). Such an approach would be a great asset to LANL. MPEAs/HEAs offer a wide space to pioneer and develop robust processes for materials-by-design.

2.2 High Explosives

The High Explosives (HE) session took place on Wednesday August 7, 2019, and was focused on modeling and experimental techniques that can address deformation mechanisms active in a few to several grains. Like the other sessions, the speakers were predominantly from academia with the exception of Lee Perry (LANL, M-7), Kyle Ramos (LANL, M-7), and Marc Cawkwell (LANL, T-1). Ramos and Cawkwell presented a joint talk on recent work being completed under a LDRD-DR. The academic speakers included: Tommy Sewell (University of Missouri), H.S. Udaykumar (University of Iowa), Weinong Chen (Purdue University), Keith Gonthier (Louisiana State University), Vikas Tomar (Purdue University), and Marisol Koslowski (Purdue University). This group encompassed expertise in state-of-the-art mesoscopic modeling and experimental techniques. The experimental and modeling efforts cover a wide range of phenomena that must be considered for HE including hot spot formation, compaction, damage evolution (fracture, debonding, etc.), pore collapse, chemistry, etc.

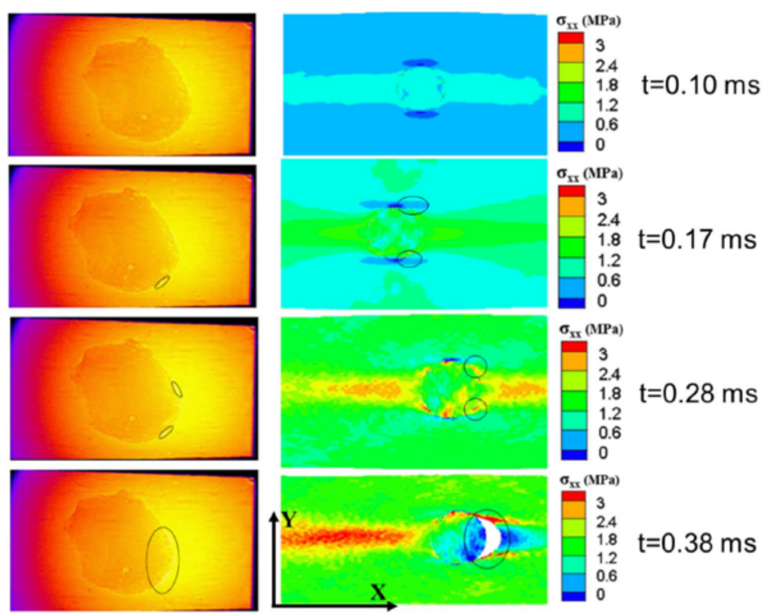

Figure 8: Interface separation of a particle in a binding agent in a Kolsky bar tension experiment (left) and simulated results for the experiment using a finite element approach (right). (C. Prakash et al. Eng. Frac. Mech. (191) 46-64 (2018)).

The talks that addressed mesoscale modeling often highlighted challenges of bridging scales. For example, Dr. Sewell presented direct comparisons between molecular dynamics (MD) and isotropic continuum models (Johnson-Cook elastic-perfectly plastic, constant specific heat to match MD). These simulations were meant to examine the temperature fields predicted with each model with an attempt to match up constitutive and equation of state (EOS) models between MD and the continuum scale. Overall, the results showed that time to collapse and temperature distributions could be reasonably matched. However elastic anisotropy could not be matched with the continuum constitutive model, and played a notable role in results at lower impact speeds. This issue of addressing anisotropic plasticity and also fracture prevailed in several of the talks presented in this session. Many (including Dr. Koslowski, Dr. Chen, and others) showed that accounting for these material behaviors had strong effects on the overall material response.

One of the most sophisticated and integrated modeling approaches currently in use in this field, SCIMITAR3D, was presented by Dr. Udaykumar. In particular, this code capability has been developed over ~15 years with the goal to simulate HE at the mesoscale. This is an Eulerian framework that operates on a fixed Cartesian grid, it includes adaptive mesh refinement (AMR) and is parallel. This approach has more recently started to apply machine learning (ML) techniques to help with the issue of bridging or blending scales. Dr. Udaykumar showed examples of starting with various microstructures, performing a multitude of simulations (600+) to 'learn' continuum reaction rates (needed for reactive burn models). While this method is both powerful and mature, the machine learning component cannot fully account for important effects naturally without further development (which are subject of current research). Although the work is 2D only, it could be extended to 3D, with increasing computational costs.

Current and Future Collaboration Opportunities

First, it is worth mentioning that the HE community had a large presence at this workshop, and is actively engaging in and open to collaboration. Several of the researchers that presented in the workshop are associated with a recent DoD Multidisciplinary University Research Initiative (MURI) award (Sewell, Udaykumar, Tomar). The MURI has a "kick-off" meeting next month (Sept. 2019), and roughly 20 people from LANL will be in attendance with the hope of fostering collaborations *at the ground level*. Importantly, since the MURI is just starting, there is a fantastic opportunity to leverage their work, funded from AFOSR, with LANL's interests (Joint Munition Program (JMP), ASC-PEM, ASC-IC, Conventional High Explosive Grand Challenge, Science Campaign 2 and others). The AFOSR is interested in HMX based explosives, which are relevant to LANL because HMX is the HE crystal in PBX 9501. AFOSR is also interested in collaboration with the National Laboratories, having students visit the labs, etc.

In addition to this potential future area for collaboration, many examples of collaboration already exist. For example, Dr. Sewell, Dr. Zhao at Missouri and Dr. Udaykumar, Dr. Rai from Iowa have active collaborations with LANL (Drs. Kober, Aslam, Cheng, Perry and Henson). Dr. Rai will join LANL as a director's postdoc in March 2020. Other collaborations exist via the Notre Dame CSWARM ASC-PSAAP-II centers (e.g., with Dr. Chen from Purdue). Also, the LDRD-DR project led by Kyle Ramos and Marc Cawkwell has collaborations with several DOD researchers, in particular at the Army Research Lab, including Dr. Rich Becker and Dr. Chris Meredith, and is seeking to develop connections with the newly established MURI team.

2.3 Surface Science

The Surface Science session was held the afternoon of Wednesday August 7, 2019. Unfortunately, the session only consisted of one speaker, Florin Bobaru (University of Nebraska, Lincoln). It is worth noting that several others in the field were contacted and invited to speak, but were unable to attend due to travel and conference conflicts. The issues of focus in this session, such as microstructural changes or changes in the material response due to corrosive environments and coupling between corrosion and grain-level deformation mechanisms, are still of great interest to Laboratory scientists. Perhaps a future workshop could have a larger focus on surface science topics, and be help at a different time of the year to encourage attendance from the community.

Dr. Bobaru presented his recent work addressing brittle cracking induced by corrosion using a peridynamics framework. Capturing such behavior is important because even relatively minor levels of corrosion can cause brittle damage and failure in materials. Peridynamics has been traditionally used to address brittle fracture at the mesoscale, and specifically crack formation in materials. Dr. Bobaru's recent work has connected this framework to corrosion induced crack formation, and in particular he presented recent results addressing pitting corrosion. Pitting corrosion is particularly important in stainless steels and aluminum alloys that are used in aerospace and naval structures, or metals used in biomedical applications. Pits in the material formed due the corrosive environment (e.g. salty environments) initiate both surface or inter-granular cracks. This coupling is accounted for in the model. It is worth noting that Dr. Bobaru mentioned that, for this field, anisotropy can have a significant effect (similar to issues discussed in the HE talks). In addition, extending the method to consider microstructure and corrosion due to radiation environments are topics of current/future work.

Current and Future Collaboration Opportunities

Due to the low turnout in speakers in this session, there was a correspondingly low turnout in LANL scientists in this field. Unfortunately, this hindered the possibilities of developing future collaborations, although Dr. Bobaru seems receptive of such a collaboration. As mentioned above, a workshop with surface science featured more prominently may be beneficial in the future.

2.4 Manufacturing

The Manufacturing session was held Thursday, August 8, 2019. This session addressed how different manufacturing techniques (e.g. casting, additive manufacturing) will impact material microstructure and the corresponding overall material response. Speakers included: Richard LeSar (Iowa State University), Suresh Babu (University of Tennessee, Knoxville), Peter Collins (Iowa State University), Amber Genau (University of Alabama at Birmingham), and Christopher Newman (LANL, T-3). The presentations focused on showing how the various parameters during solidification (such as geometry, cooling rate, chemical composition) affect the resulting microstructure and how this knowledge could inform the design of "customized" materials (e.g. hybrid materials). The lack of in-situ and dynamic experimental techniques, in particular for casting, was brought-up during the discussion. The main focus of this session, however, was on additive manufacturing (AM), and both modeling and experimental approaches to address this complex process.

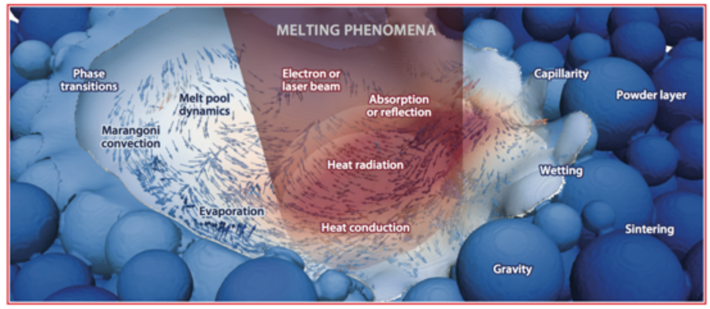

Figure 9: Physical phenomena that occur during laser/electron beam melting of a powder bed. (Markl and Körner, Annu. Rev. Mater. Res. (46) 93-123 (2016)).

Dr. LeSar (modeling perspective) and Dr. Collins (experimental perspective) are working collaboratively to study the drastic changes in microstructure due to processing with AM. To fully understand this process there is a wide range of physical processes that must be considered including microstructure, heat transfer, solidification, and chemistry (see Figure 9). Rather than trying to accurately consider all of these processes, Dr. LeSar and Dr. Collins decided to aim for 'an 80% solution' instead. With this approach, Dr. Collins showed that composition, for example, contributes ~70-80% to the yield strength, while texture only has a ~0-10% contribution. This, and similar information, has allowed them to reduce the time from design to delivery for large components for customers (down to ~3 months). Thinking back to points raised by Dr. Sarrao and the goals of DMMSC, this type of approach and analysis could help to streamline new concepts and new materials making them readily available to the DOE Laboratories in relative short timeframes.

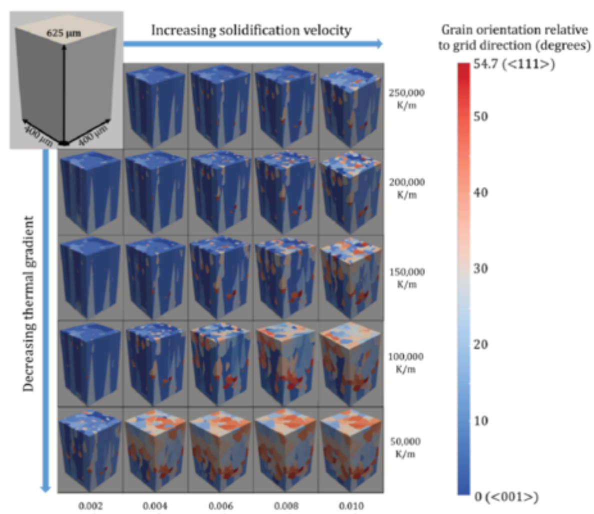

Figure 10: 3D modeled microstructures under constrained alloy solidification conditions. The effects of varying the thermal gradient and solidification rate on the microstructure is shown. (M. R. Rolchigo and R. A. LeSar. Comp. Mater. Sci. (163) 148-161 (2019)).

Current and Future Collaboration Opportunities

As in the other areas covered in the workshop, there are current collaborations in the area of manufacturing. For example, Dr. LeSar has active collaborations with colleagues at LANL, including Laurent Capolungo (LANL, MST-8) the PI of a recently awarded LDRD-DR project starting in FY20.

2.5 Poster Session

The poster session was held Tuesday (August 6, 2019) in the evening, and consisted of ~16 posters presented by LANL scientists and students, and also attendees from academia. These posters spanned the topics of the workshop including titles such as:

- *Statistically informed effective moduli model for damage in quasi-brittle materials under high rate loading conditions* (Kevin Larkin, New Mexico State University)
- *Multimaterial Closure Model Behavior During Shock Deformations* (Conant Kumar and Christopher Coffelt, XCP Summer Workshop Students)
- *Effect of reaction kinetics models on simulation of hotspot initiation and growth in HMX* (Nirmal Rai, University of Iowa)
- *Tracking Hot Spot Growth and Temperatures in a Model Plastic-Bonded Explosive Under Shock Compression* (Belinda Pacheco, University of Illinois)
- *Advances in Constitutive Modeling for Simulated Imaging from Dynamic XFEL Experiments* (D.J. Luscher, LANL)
- *Grain-size effects in the shock heating of idealized PBXs* (Nisha Mohan, LANL)
- *Modeling and Simulation Capability Development in Support of Additive Manufacturing for ECP and PEM* (Christopher Newman, LANL)

In particular, topics in the Metals and High Explosives sessions were well represented in the poster session by LANL attendees. ASC-PEM, both the Materials and the High Explosives Project, had posters presenting recent and ongoing work addressing modeling and experimental needs at the mesoscale. In addition, the LANL LDRD-DR project (PI: Ramos) was represented, in addition to work associated with the newly awarded MURI project (Dr. Sewell) investigating High Explosives.

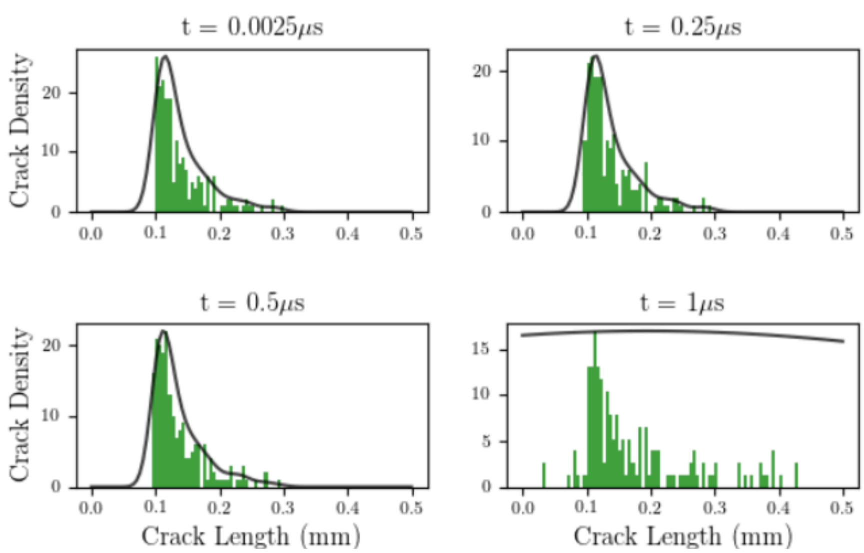

Figure 11: Evolution of crack length statistics over time during a Be-Be flyer plate simulation (figure courtesy of Kevin Larkin).

3. Recommendations and Conclusions

Clearly much is going on in the mesoscale science community both internally at LANL and externally within academia. With so much out there, one big issue is how to focus and apply LANL's efforts to make the most of our funding and, more importantly, our scientists' time, effort and expertise, so that this work can have a large impact on mission-related problems. Of course, one way to optimize this is to build strong collaborative efforts with those in academia working on similar problems. Our investment in collaboration should balance several objectives:

1. Training and recruitment of the future LANL scientific workforce.
2. Optimally engage in areas with high LANL impact, where university collaborations can enhance the development of our in-house capabilities.
   - It is worth noting that there are funding opportunities for academia put out by DOE (and NNSA), which typically focus on research activities motivated by DOE-NNSA needs (e. g., the recent DOE-NNSA call for Stewardship Science Academic Alliances Program Center of Excellence for Property of Materials under Extreme Conditions – DE-FOA-0002149). These opportunities strongly encourage collaborations with the DOE Labs, and even accept letters of support as part of the proposal from Laboratory personnel. However, Laboratory personnel are not eligible for funding through these opportunities. If Laboratory personnel could receive funding through such calls, use and development of LANL's (appropriate) in-house capabilities could be specifically defined in the project scope. Besides directly engaging LANL's tools, this would allow for stronger collaborations since LANL scientists would have more time to engage in the work. This would also allow for students to start learning and working with LANL resources earlier, which would both attract and engage the high-quality candidates needed for our future workforce.
3. To out-source complementary research activities where we simply are not going to develop the requisite expertise.
   - One example of where LANL and universities have complementary goals may be on the experimental front. During the workshop, several professors brought up issues of needing to have the ability to complete experiments quickly so that students can get and analyze enough data in a relatively quick time frame. This is largely motivated by the fact that students must be able to complete enough work for a thesis in a reasonable amount of time for graduation. This has resulted in a number of 'table-top' experimental systems, that can produce results quickly although typically at reduced resolution. LANL should rely on universities to fill such a need (i.e., quick throughput experiments), and instead focus their efforts and funding on higher resolution techniques and facilities.

Another recommendation is that LANL should direct research efforts that are specifically focused on solving specific mission-related problems. Advancing the scientific understanding of how materials deform from a mesoscale perspective presents a huge canvas of research opportunity which in turn begins to define several research challenges. The scientific challenges of this endeavor are so vast, that it may behoove us to adopt a top-down strategy for prioritization, in which we first identify the driving macroscale problems that will benefit from mesoscale information. Exemplar problems are discussed in the addendum to this report.

Finally, possible focuses for future mesoscale science workshops:

- A workshop with more focus on surface science may be beneficial since this community was a bit under-represented in this workshop. This was partially due to the timing of the workshop, which seemed to conflict with a number of other meetings in this community. Corrosive environments (including radiation environments) are of interest to LANL, and a detailed look at mesoscale science in this area could highlight both needs and opportunities.
- A workshop focused on code development aspects, particularly looking from the top down. What numerical techniques, challenges, opportunities exist to incorporate mesoscale information into larger length scale models (particularly hydrocodes)?
- A workshop focused on validation and verification of mesoscale models, again with focus on the connection to larger length scale models. How would this be done and where are there information gaps (e.g., where are there gaps in needed experimental evidence)?
- A direct follow-on to this workshop, which could continue the discussions and collaborations enhanced with this workshop. Overall, the community responded very positively to this workshop, making it a success. To enhance a follow-on workshop, some discussion on funding opportunities, sub-contract processes, student intern opportunities could be included to both educate and enhance collaborations.

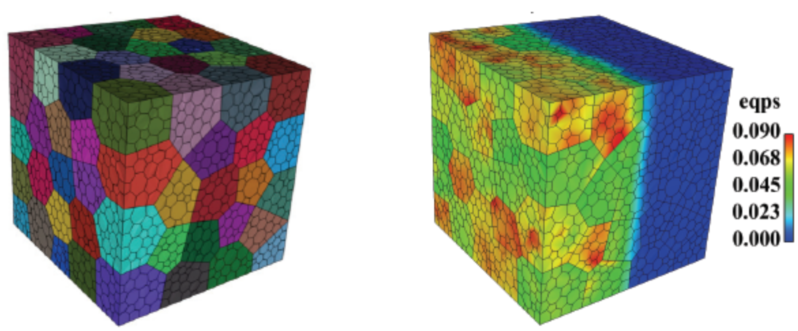

Figure 12: A 3D simulation of the dynamic response of polycrystalline cooper using a crystal plasticity model implemented in the ASC hydrocode FLAG (D. J. Luscher, et al. AIP Conf. Proc. (1979) 180006 (2018)). The polyhedral mesh (left) and the equivalent plastic strain after impact (right) is shown.

4. Speaker Abstracts

4.1 Defective Metals

The Role of Elastic and Plastic Anisotropy in Ductile Damage Nucleation along Grain Boundaries

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ABSTRACT- Recent mesoscale experimental observations of dynamic ductile failure by Wayne et al. [2010] and Brown et al. [2015] have demonstrated a strong relationship between grain boundary (GB) misorientation and the likelihood of failure initiation along said GB. This correlation has been attributed to inherent GB weakness of particular misorientation. Here we discuss the role played by mechanics, i.e. elastic and plastic anisotropy, on the experimental observation of Wayne et al. [2010] and Brown et al. [2015]. We make use of a recently developed framework for modeling dislocation-based crystal plasticity and ductile failure of single crystals under dynamic loading (CPD-FE) proposed by Nguyen et al. [2017]. Polycrystals are studied at the mesoscale level through the explicit resolution of individual grains, i.e. resolving each individual grain's size, shape, and orientation. In our simulations, failure naturally localizes along the GBs with no necessity for ad hoc rules governing damage nucleation. We carry out a few thousand mesoscale calculations, systematically varying the misorientation angles of the GB in the computational microstructure. Despite the fact that we neglect the possibility of variations in inherent GB weakness, our simulations agree favorably with the experimental observations, implying that stress concentration generated by elastic and plastic anisotropies across GBs is a dominant governing factor in this phenomenon. Lastly, we find that misorientation angle is an insufficient GB descriptor to predict the likelihood of intergranular spall failure, which is better understood through the consideration of additional GB degrees of freedom.

Acknowledgement: The work was performed under the auspices of the U.S. Department of Energy under contract DE-AC52-06NA25396 and partly under sub-contract 464745. The material is also based upon work supported by Army Research Laboratory under the MEDE Collaborative Research Alliance through Cooperative Agreement Number W911NF-12-2- 0022.

REFERENCES:

1. L. Wayne, K. Krishnan, S. DiGiacomo, N. Kovvali, P. Peralta, S. Luo, S. Greenfield, D. Byler, D. Paisley, K. McClellan, A. Koskelo, R. Dickerson, 2010, "Statistics of weak grain boundaries for spall damage in polycrystalline copper", Scr. Mater. **63** (11), 1065-1068.

2. A.D. Brown, L. Wayne, Q. Pham, K. Krishnan, P. Peralta, S.-N. Luo, B.M. Patterson, S. Greenfield, D. Byler, K.J. McClellan, et al., 2015, "Microstructural effects on damage nucleation in shock-loaded polycrystalline copper", Metall. Mater. Trans. **46** (10), 4539-4547.
3. T. Nguyen, D. Luscher, J. Wilkerson, 2017, "A dislocation-based crystal plasticity framework for ductile failure of single crystals", J. Mech. Phys. Solid. **108,** 1-29.

Non-Destructively Probing Mesoscale Radiation-Induced Microstructural Evolution

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ABSTRACT - Nuclear materials age in service, with their properties changing as a combined result of how they were produced and to what they were exposed. This aging, which can be due to a combination of thermal and irradiation origins, sometimes results in degraded performance which can lead to failure. It also often leaves fingerprints, measurable either directly or indirectly. In this talk we will explore the use of transient grating spectroscopy (TGS) [8], a picosecond ultrasonic non-destructive technique, as a method to both assess the health of key light water and fast reactor components due to spinodal decomposition, short range ordering, void swelling, and phase precipitation, and to reconstruct their irradiation history. Changes in thermal [3], elastic [5], and acoustic material properties are indirectly linked to the quantities of interest, such as Charpy impact energy via surface acoustic wave peak splitting for structural materials, void swelling [1] and defect clustering [7] in single crystal metals via thermo-elastic property response, and irradiation dose history to reconstruct reactor usage, particularly for additively manufactured materials. This wide variety of examples highlights the vast, unexplored space where non-destructive, indirect, mesoscale measurement techniques can far more rapidly uncover new science and assist industry in nuclear materials forensic and health assessment issues.

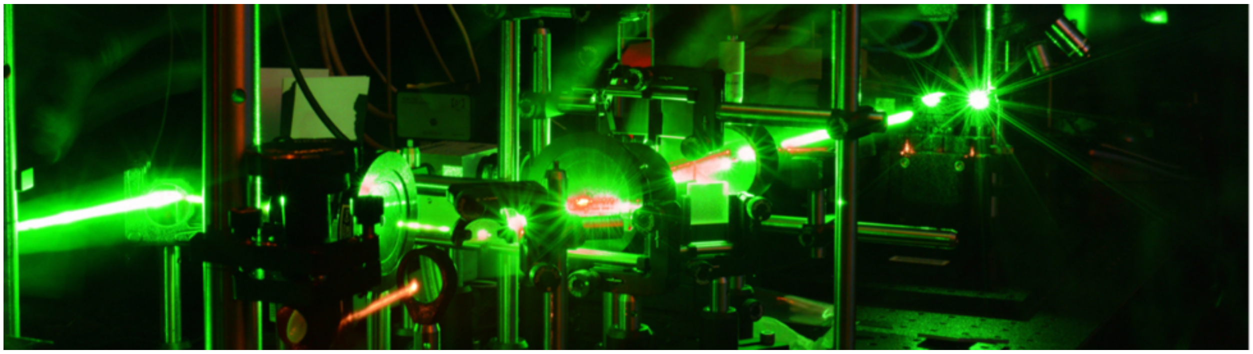

Figure 1: A long-exposure photograph of our TGS facility at MIT, with pump (green) and probe (red) lasers

A number of studies will be presented along this theme, demonstrating the utility of this new technique for radiation materials science. We will specifically show how changes in surface acoustic wave (SAW) speed, which directly link to Young's Modulus and Poisson's ratio, can identify the radiation dose in DPA to the onset of void swelling in single crystal copper [1] and nickel [6]. Radiation-dependent changes in thermal diffusivity help show the saturation of radiation-induced dislocations and defect clustering in single-crystal niobium irradiated with Si ions [7], while the same thermal diffusivity changes reveal the onset and saturation of radiation induced segregation in neutron-irradiated 304 stainless steel to 28 DPA. Finally, a number of studies, ranging from deducing thermal properties of irradiated carbon nanotube coatings [2], MAX phase materials, tungsten fuzz development for fusion applications, and illustrating temperature-dependent radiation effects in SiC will be shown to show the broad applicability of TGS [8].

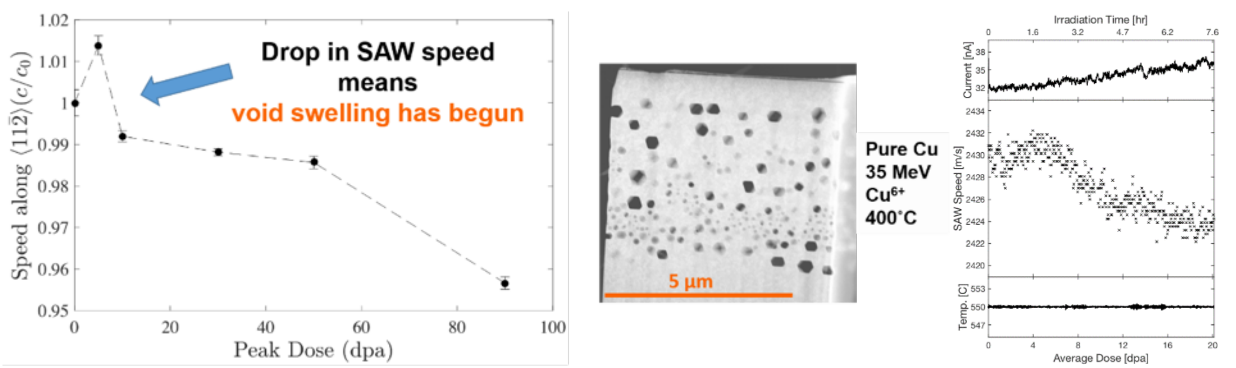

Figure 2: Drop in SAW speed (left) corresponding to the onset of void swelling in single crystal copper (center, [1]), and *in situ* detection of the same in single crystal nickel (right, [6])

References

1. Dennett, C. A. et al. "Detecting self-ion irradiation-induced void swelling in pure copper using transient grating spectroscopy." *Acta Mater.* **145**:496-503 (2018).

2. Cometto, O. et al. "A thermal study of amorphous and textured carbon and carbon nitride thin films via transient grating spectroscopy." *Carbon* **130**:355-361 (2018).

3. Dennett, C. A., Short, M. P. "Thermal diffusivity determination using heterodyne phase insensitive transient grating spectroscopy." *J. Appl. Phys.* **123**:215109 (2018).

4. Dennett, C. A., Short, M. P. "Time-resolved, dual heterodyne phase collection transient grating

spectroscopy." *Appl. Phys. Lett.* **110**:211106 (2017).
5. Dennett, C. A. et al. "Bridging the gap to mesoscale radiation materials science with transient grating spectroscopy." *Phys. Rev. B* **94**:214106 (2016).
6. Dennett, C. A., Buller, D., Hattar, K., Short, M. P. "Real-time thermomechanical property monitoring during ion beam irradiation using in situ transient grating spectroscopy." *Nucl. Instrum. Meth. B* **440**:126-138 (2019).
7. Ferry, S. E., Dennett, C. A., Woller, K. B., Short, M. P. "Inferring radiation-induced microstructural evolution in single-crystal niobium through changes in thermal transport." *J. Nucl. Mater.* (In Press) (2019).
8. Hofmann, F., Short, M. P., Dennett, C. A. "Transient grating spectroscopy: An ultrarapid, nondestructive materials evaluation technique." *MRS-B* **44**:392-402 (2019).

4.2 Multiple Principal Element/High Entropy Alloys

Metastable high entropy alloys in extreme environments

Shaolou Wei, Motomichi Koyama, Seyedeh Mohadeseh Taheri-Mousavi, Haoxue Yan, Jinwoo Kim, Benjamin Clive Cameron, Sina Moeini Ardakani, Nobuhiro Tsuji, Ju Li, Cemal Cem Tasan

ABSTRACT - Here we present two interesting observations in a metastable high entropy alloy: (i) in presence of hydrogen, and (ii) at severe deformations.

Designing an *in-situ* electron channeling contrast imaging experiment, we show micron-range dislocation activity during hydrogen desorption from HEA samples under no external stress. Combining grand canonical Monte Carlo, molecular dynamics, and finite element simulations, we reveal that the required shear stress arises from grain boundary hydrogen segregation. Evidently, rather than causing the classical dislocation pinning effect, hydrogen facilitates dislocation motion by generating segregation-induced stresses.

In the second part, we will demonstrate that the parent-FCC phase in the same HEA can exhibit the strain-induced HCP-martensitic transformation, and the resulting HCP phase can further transform, activating thus a mechanically-induced FCC-HCP-FCC dual-TRIP effect, upon severe deformation. With the aid of *in-situ* synchrotron X-ray diffraction, integrated SEM/EBSD, and microstructural-based strain mapping techniques we reveal the corresponding deformation micro-mechanisms including transformation kinetics, kinematics, and global-local strain evolution. We will show that this sort of dual-TRIP mechanism exhibits a desirable potential to overcome the inherent property improvement limit of classical-TRIP effect.

Phase field dislocation dynamics for BCC MPEs

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ABSTRACT - Refractory multi-principle element alloys show great potential for high-temperature applications, but their deformation mechanisms are not well understood. Since deformation of these materials in mediated by slip, there is a strong motivation to understand dislocation behavior in these alloys. To study this, we develop a phase field dislocation dynamics (PFDD) model. Because screw dislocations are known to dominate behavior in BCC metals, a dislocation character dependence is added to the PFDD model by adjusting the lattice energy, which accounts for the dislocation cores. Additionally, the random chemical variations of the disordered solid solution phase are modelled via a position-dependent lattice energy. This model can be applied to a ternary MoNbTi alloy by incorporating the distribution of DFT-calculated unstable stacking fault energies. The results of this model on the behavior of Frank-Read sources will be presented.
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Multi-Principal Element Alloys for Performance in Extreme Environments

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ABSTRACT - Multi-principal element alloys (MPEAs), without a primary alloying addition like conventional alloys, are stimulating the exploration of novel alloying, microstructure, and property designs. Although MPEAs with remarkable properties have been reported, the focus to date has primarily been on the quest for single-phase, equiatomic alloys that exhibit solid solution strengthening.

Yet, opportunity exists to find non-equiatomic alloys with maximized solid solution strengthening and non-equiatomic alloys with multi-phase microstructures that exhibit additional strengthening mechanisms. Here we focus on high-throughput, thermodynamic modeling to predict non-equiatomic Co-Cr-Ni alloys that exhibit TRansformation Induced Plasticity (TRIP) and/or TWinning Induced Plasticity (TWIP) to improve toughness for blast resistance. We also study TRIP/TWIP in lightweight metallic alloys such as Ti, important for aerospace, defense, and biomedical applications. We seek to fundamentally understand TRIP/TWIP deformation mechanisms by in-situ synchrotron x-ray imaging and/or diffraction during quasi-static and/or dynamic compression and tensile testing, along with complementary ex-situ microstructural and mechanical characterization, to ultimately tailor microstructural and mechanical response.

Metastabilty Driven Hierarchical Microstructural Engineering of Complex Concentrated Alloys for Extreme Conditions

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ABSTRACT - Complex concentrated alloys (CCAs) extend the compositional paradigm shift of high entropy alloys (HEAs) to new microstructural opportunities. CCAs provide opportunities for tunable performance by manipulating deformation mechanisms. We have studied $Al_xCoCrFeNi$ and Fe-Mn-Co-Cr-Si alloys that exhibit potential for a combination of phase transformation and twinning. These alloys give greater flexibility for tailoring transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP), which have guided design of next-generation steel alloys over the last 20 years to a new level. For TRIP CCAs, the ductility can be extended to as high as 50% while maintaining a strength exceeding 1 GPa. On the other hand, hierarchical microstructural engineering in $Al_xCoCrFeNi$ alloys can lead to over 2 GPa strength and >10% ductility. To reveal the underlying mechanisms governing the material's fracture, a suite of quasistatic and dynamic tests were performed. The Fe-Mn-Co-Cr-Si alloys were shown to exhibit extensive gamma (f.c.c.) to epsilon (h.c.p.) phase transformation followed by additional twinning in the epsilon phase. Design of non-equiatomic CCAs provides a vast, and vastly unexplored compositional space for developing new alloys with tunable properties. This "Microstructural Flexibility" in alloys can be very useful for overcoming the conventional strength-ductility paradigm that limits current dynamic performance of metals. Although these alloys exhibit large uniform ductility, the non-uniform ductility is quite limited. The non-uniform ductility represents strain for growth of voids and ductile fracture. These aspects will be reviewed and the differences from conventional deformation and ductile fracture will be highlighted.

4.3 Phase Transformations

Modeling the alpha/omega thermal stability in shocked Zr: A coupling between dislocation removal and phase transformation

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ABSTRACT - Under high pressure, Zr undergoes a transformation from its ambient equilibrium hexagonal close packed α phase to a simple hexagonal ω phase. Subsequent unloading to ambient conditions does not see a full reversal to the α phase, but rather a retainment of significant ω. Previously, the thermal stability of the ω phase was investigated via in-situ synchrotron X-ray diffraction analysis of the isothermal annealing of Zr samples shocked to 8 and 10.5 GPa at temperatures 443, 463, 483, and 503 K. The phase volume fractions were

tracked quantitatively and the dislocation densities were tracked semi-quantitatively. Trends included a rapid initial (transient) transformation rate from ω→α followed by a plateau to a new metastable state with lesser retained ω (asymptotic). A significant reduction in dislocation densities in the ω phase was observed prior to initiation of an earnest reverse transformation, leading to the hypothesis that the ω→α transformation from is being hindered by defects in the ω phase. As a continuation of this work, we present a temperature dependent model that couples the removal of dislocations in the ω phase and the reverse transformation via a barrier energy that is associated with the free energy of remaining dislocations. The reduction of dislocations in the ω phase occurs as a sum of glide and climb controlled processes, both of which dictate the transient and asymptotic behavior of the annealing process respectively.

In addition, we will briefly present a new experimental technique for producing high quality planar shock impacts in the laboratory called vaporizing foil actuation. This technique is based on the exploding conductor phenomena has been demonstrated by producing like metal Zr impacts of up to 2 km/s. The instrument is fully instrumented with PDV to monitor both the flyer velocity and planarity and to perform free-surface velocimetry on the shock specimen.

Probing Phase Transformations and Twinning Across Length Scales Using 3D X-Ray Microscopy

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ABSTRACT - This talk will include the current status of three-dimensional X-ray diffraction microscopy techniques including microcomputed tomography, near- and far-field high-energy diffraction microscopy, and dark-field X-ray microscopy. These techniques offer the capability to directly observe the deformation and microstructure evolution inside bulk materials in situ and across several orders of magnitude in length scale (nanometers to millimeters). Quantities of measure include the grain map and the grain-averaged location, crystallographic orientation, elastic strain tensor, phase fraction, and active slip systems, as well as subgrain- level misorientation and lattice strain spread. These capabilities will be illustrated using numerous examples with an emphasis on research involving twinning and phase-transforming materials. Potential improvements to the time resolutions of these techniques for investigations of dynamic processes will be discussed.

4.4 High Explosives

Tandem molecular dynamics and continuum studies of shock-induced pore collapse in TATB*

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ABSTRACT - All-atom molecular dynamics (MD) and Eulerian continuum simulations, performed using the LAMMPS and SCIMITAR3D codes, respectively, were used to study thermo-mechanical aspects of shock-induced pore collapse in single crystals of TATB initially at 300 K. A cylindrical pore, with initial diameter 50 nm, was located at the center of a sample that was 150 nm ´ 150 nm along two edges. The continuum simulations were precisely 2D whereas the MD simulations were "quasi-2D" with a thickness of »3.5 nm in the third direction. Three impact speeds—0.5 km s^{-1}, 1.0 km s^{-1}, and 2.0 km s^{-1}—were used to generate the shocks. These impact conditions are intuitively expected to yield collapse mechanisms ranging from predominantly visco-plastic to hydrodynamic-like.

For the MD studies, three crystal orientations (i.e., shock-propagation directions) were studied that span the limiting cases with respect to the crystal anisotropy in TATB. For the continuum simulations an isotropic constitutive model was used; thus, crystal anisotropy effects are absent. The continuum simulations were performed for two cases: a "classical" (i.e., temperature-independent) specific heat corresponding to that in the MD studies, thereby allowing for the closest comparison between the atomistic and continuum predictions; and a temperature-dependent specific heat that captures the quantum-mechanical behavior of that property. Two different models for the melt curve were also studied in the continuum case: one using a constant, normal- melting-point value from experiment; and one that uses a pressure-dependent melt curve, calculated using MD for pressures up to 2 GPa and then extrapolated to higher pressures using a Simon-Glatzel fitting form.

The evolution of spatio-temporally resolved properties during collapse, simulated using both MD and continuum mechanics, will be presented and discussed both qualitatively and quantitatively. Among the properties of interest during collapse are 2D spatial distributions of local temperature, stress, pore size and shape, and flow properties. Time-position (t-z) diagrams of some of those same properties will also be discussed, focusing on a thin strip of material along the centerline of the pore and parallel to the shock direction. Additionally, histograms of local temperature and pressure at times just following pore closure will be shown.

As one might expect, the MD simulations reveal considerable orientation dependence and anisotropy during pore collapse, especially for the weaker shocks for which the material properties are more important. Within the isotropic elastic/perfectly plastic continuum framework used, and for the range of impact conditions studied, the specific heat sub-model exerts far more influence on the continuum predictions than does that for the melt curve. Treating the MD predictions as 'ground truth', albeit with a classical rather than quantum-like heat capacity, it will become clear that extension of the constitutive model to account for crystal anisotropy effects will be required to achieve a high-fidelity continuum mechanical description of pore collapse in TATB.

* Research performed with support from the U.S. Air Force Office of Scientific Research 'Dynamic Materials and Interactions' portfolio; Dr. Martin J. Schmidt, program officer.

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SCIMITAR3D: A sharp-interface eulerian framework for multi-scale modeling of energetic materials

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ABSTRACT - Energetic materials (propellants, explosives, pyrotechnics) are typically organic crystalline solids that, upon application of sufficiently strong loads, release large amounts of energy on short time scales. The initiation sensitivity of such materials arises due to energy localization by shock focusing at pores and other internal defects; the resulting hotspots grow to rapidly consume the surrounding material leading to detonations. Among the possible mechanisms of hotspot induced initiation, plastic deformation, frictional heating at particle-particle interfaces and fracture can all play significant roles. This talk will summarize the development of SCIMITAR3D—a computational code and framework for multi-scale modeling of energetic materials performance. The capabilities of the code to proceed from imaged microstructures to uncertainty quantified meso-informed performance prediction of shock-loaded energetic materials will be outlined. Recent work on crystal plasticity based and phenomenological rate dependent plasticity models and their implications for predicting the response of energetic crystals to high strain rate (shock) loading will also be presented. Insights from MD simulations will be combined with those from continuum models. Outstanding research issues and directions for future work will be pointed out.

Real-time visualization of meso-scale damage evolution in energetic materials under impact

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ABSTRACT - For energetic materials under impact loading, the meso-scale, granular-level deformation, damage, and failure processes are critical factors affecting the sensitivity of the materials. Thus, it is desired to track the damage initiation and evolution in real time during the dynamic deformation of the specimens at this scale. We integrated the high-speed X-ray imaging capabilities present at the Advanced Photon Source beamline 32 ID-B (Argonne National Laboratory) with the high-rate loading offered by the Kolsky compression/tension bar and light gas gun. High-speed X-ray images and X-ray diffraction can be obtained simultaneously. These new experimental capabilities were applied to study the energetic crystal damage and cracking processes, crystal-binder interfacial debonding behavior, and the effects of initial defects inside the energetic crystals on the failure behavior of energetic materials under impact. To record the initial microstructure and defect distribution, the specimens were characterized with X-ray computed tomography before impact experiments.

Presenting author: Wayne Chen

Mesoscale Informed Ignition and Burn Models for Weak Shock Initiation of Porous HE

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ABSTRACT - Deflagration-to-Detonation Transition (DDT) in confined, porous high-explosive occurs by a complex mechanism that involves compaction shock interactions within the material. Piston driven DDT experiments indicate that detonation is abruptly triggered by the interaction of a strong burn-supported secondary shock and a piston-supported primary (input) shock, where the nature of the interaction depends on initial packing density and primary shock strength. These interactions influence transition by affecting hot-spot formation during pore collapse. A hot-spot based Ignition and Burn (I&B) model is formulated for porous HMX that is conceptually similar to conventional I&B models but describes ignition in terms of a pressure-dependent hot-spot formation rate and burn in terms of a dissipation-dependent regression rate that notionally accounts for hot-spot facilitated burn induced by strong shocks. Mesoscale simulations are performed to characterize hot-spot fields within shocked porous explosives and to guide development of the I&B model. The model predicts features representative of a Type-I DDT mechanism that is typical of weak shock initiation of porous explosive. The mechanism involves internal formation of a secondary compaction shock that can appreciably affect wave dynamics by inhibiting gas permeation and reaction provided that local dissipation is insufficient to trigger hot-spot facilitated burn. Predictions indicate conditions favorable for the formation of fast propagating, spontaneous combustion waves that are influenced by shallow spatial gradients in volume fraction behind the secondary shock.

Interface Level Stress Measurements for Describing HE Material Mesoscale Response under Impact Loading

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ABSTRACT - Role of interfaces at high strain rates approaching shock loading in materials is a challenging problem to solve. Under shock loading one can use an equation of state to describe overall homogeneous material behavior. At non-shock high strain rate loads one can use viscoplasticity driven constitutive models to describe material behavior. However, as one dives deeper into analyzing a material response to high strain rate loading, at the localized scale of interfaces local strain rates and strains are significantly different from globally applied strain rates. As such locally material can deform in significantly different and unexpected ways than what is expected using a localized homogeneous equation of state or a viscoplasticity model. This issue bears significant attention when one might want to change localized chemistry/chemical

composition of materials to change overall response to impact loading. Interfacial Multiphysics Lab (IML) at Purdue has been performing time resolved interface level stress and thermal measurements under impact loading using nanomechanical Raman spectroscopy coupled with numerical advancements in the cohesive finite element method. IML measurements have lead to first ever measurements of interface level shock viscosity that defines a new way to identify local shock fronts at microstructural scale. It is found that chemical composition can significantly alter local shock front. In addition, a new approach to measure effect of high strain rate on interface level constitutive confinement effect has been developed. It is shown localized confinement alters from being additive in Prager type models to multiplicative under high strain rate loading. A modified Johnson-Cook model is presented that is validated based on local microstructurally measured experimental data.

Dynamic response of high energy materials

Marisol Koslowski

ABSTRACT - Polymer bonded explosives consist of high energy particles in a polymeric binder. When these composites are subjected to heat, impact, or other stimulus they may undergo a rapid chemical change. This process is controlled by the formation of high temperature localized regions known as “hot spots”. The mechanisms of hot spot nucleation are controlled by the microstructure, for example in the same sample some particles ignite while others do not.

The sensitivity of the microstructure to initiation is studied with finite element simulations. The results help to identify the mechanisms of hot spot formation under a range of mechanical stimulus. The finite element model incorporates anisotropic plasticity and fracture and heat transport using a phase field approach. Microstructures with different initial defects, including cracks, debonding and voids are analyzed. Furthermore, we analyze the relative importance of plastic dissipation and friction for different crystal orientations and grain sizes.

Mesoscale Mechanics of Energetic Materials: A coordinated experiment-theory effort using new in situ probes

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ABSTRACT - Weak impacts on high explosives (HE) can give rise to either violent reactions or harmless fracture and material dispersal. Predicting this response or the state of damage in the material remains an unsolved technical challenge. In situ mesoscale insights to anisotropic dislocation-mediated plasticity, phase transitions, and damage are needed to quantify fundamental structure-property relationships, inform theory, and enable high fidelity simulations.

Time-resolved, in situ X-ray diffraction and phase contrast imaging during dynamic loading has been performed for single crystal and plastic bonded formulations of cyclotrimethylene trinitramine (RDX), cyclotetramethylene tetranitramine (HMX), and pentaerythritol tetranitrate

(PETN). Laser-driven shock, gas gun, and Split Hopkinson Pressure Bar (SHPB) experiments have been performed to span multiple orders of strain rate, using synchrotron (Advanced Photon Source) and X-ray free electron laser (Linac Coherent Light Source) radiation.

Multiphase single crystal plasticity models have been developed. They consist of non- linear thermo-elasticity with the purely volumetric portion replaced with a Helmholtz free energy equation-of-state (EOS) assuming a two-temperature Debye model. Mobile and immobile dislocation density kinetics are described by the Orowan expression for slip rate using the Austin-McDowell model for dislocation velocity. Multiphase EOS were constructed from pressure-density isotherms while imposing the temperature-presssure dependence of the transition through Gibbs free-energy. Constitutive equations were parameterized with: i) two-temperature Debye model EOS using vibrational modes calculated using DFT-D3 (BJ), ii) experimental elastic constants and their temperature derivative, iii) pressure derivative of elastic constants from atomistic calculations, iv) all slip systems from experiments, and v) the plasticity models were fit to velocimetry data from a small subset of available plate impact experiments. Remarkably these multiphase, single crystal plasticity models are capable of predicting anisotropy, thickness, and pressure dependent effects.

Combining the new experimental and theoretical capabilities, the mesoscale mechanics can be investigated at the average lattice response scale. Diffraction patterns quantify the average lattice response during elastic-plastic and phase transition and allow for direct comparison of experiments and simulations through measured and computed diagnostics.

4.5 Surface Science

Peridynamic models for corrosion damage: the role of the embrittled layer in stress corrosion cracking

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ABSTRACT - The complex interactions between corrosion damage and fracture mechanisms and their combined effect on materials' structural integrity have been long-standing open problems. Microstructural changes induced by corrosion processes through a layer near the surface lead to higher porosity and lower ductility, and are independent from hydrogen embrittlement. Such changes have a dramatic effect on ductility reduction and can easily lead to fracture and failure of loaded systems exposed to corrosive environments.

A primary reason for the slow progress in modeling of corrosion damage processes has been the major difficulties in coupling electrochemical anodic dissolution of materials with mechanical damage that quantifies the structural integrity. We recently have introduced novel peridynamic-based models for corrosion damage that have allowed, for the first time, computational predictions of pitting corrosion damage in three-dimensions with fine details that match

experimental observations over different time scales. The peridynamic (PD) model for corrosion damage couples diffusion, phase change, and mechanical damage (induced by the chemical attack). The primary reasons for the success of this modeling approach are: (a) the layer at the corrosion front that suffers degradation and embrittlement is intrinsic in the PD model, and (b) nonlocal/PD modeling allows for integrating small-scale effects (e.g. microstructure-dependent behavior) into a larger-scale homogenized, nonlocal response. Since corroded areas serve as initiation points for cracks, a coupled PD model for corrosion and fracture extends the benefits of PD modeling demonstrated in predicting fracture phenomena.

Modeling complicated couplings between corrosion and grain-level deformation mechanisms and simulating the evolution of these phenomena becomes possible in peridynamics.

References

1. S. Jafarzadeh, Z. Chen, F. Bobaru, "Computational modeling of pitting corrosion ", Corrosion Reviews, (2019). https://doi.org/10.1515/corrrev-2019-0049
2. S. Jafarzadeh, Z. Chen, J. Zhao, F. Bobaru, "Pitting, lacy covers, and pit merger in stainless steel: 3D peridynamic models", Corrosion Science, 150:17-31 (2019). https://doi.org/10.1016/j.corsci.2019.01.006
3. S. Jafarzadeh, Z. Chen, F. Bobaru, "Peridynamic Modeling of Intergranular Corrosion Damage", Journal of The Electrochemical Society, 165(7): C362-C374 (2018). https://doi.org/10.1149/2.0821807jes
4. S. Li, Z. Chen, L. Tan, F. Bobaru, "Corrosion-induced embrittlement in ZK60A Mg alloy", Materials Science and Engineering A, 713: 7-17 (2018). https://doi.org/10.1016/j.msea.2017.12.053
5. S. Jafarzadeh, Z. Chen, F. Bobaru, "Peridynamic modeling of repassivation in pitting corrosion of stainless steel", Corrosion, 74(4): 393-414 (2018). http://corrosionjournal.org/doi/abs/10.5006/2615
6. Shumin Li, Ziguang Chen, Fei Wang, Bai Cui, Li Tan, Florin Bobaru, "Analysis of Corrosion-Induced Diffusion Layer in ZK60A Magnesium Alloy", Journal of The Electrochemical Society, 163(13): C784-C790 (2016). doi: 10.1149/2.1001613jes
7. Z. Chen, G. Zhang, F. Bobaru, "The Influence of Passive Film Damage on Pitting Corrosion", Journal of The Electrochemical Society, 163(2), C19-C24, (2016). http://dx.doi.org/10.1149/2.0521602jes
8. Z. Chen, F. Bobaru, "Peridynamics modeling of pitting corrosion damage", Journal of the Mechanics and Physics of Solids, 78: 352–381 (2015). http://dx.doi.org/10.1016/j.jmps.2015.02.015

4.6 Manufacturing

Modeling the effects of alloying on microstructure formation under additive manufacturing conditions

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ABSTRACT - The work in this talk was developed as part a multi-university program focused on designing metallic alloys to take advantage of the unique processing conditions in additive manufacturing (AM) to create materials with specified microstructures, and therefore, properties. Our part of that effort was to build multiscale modeling tools to predict those microstructures. These tools require models for both alloy solidification and for the processing conditions. In our approach, we chose to focus on tools that could be used by process engineers to tune materials for their applications. As such, heat transport, melting, solute transport, and fluid flow are modeled at the macroscale via the Lattice Boltzmann method, accounting for laser absorption, Marangoni flow, and so on in the melt pool. At the microscale, alloy solidification is modeled using cellular automata models, with temperature and fluid flow boundary conditions passed from the macroscale, enabling the linking of process parameters, melt pool conditions, alloy thermodynamics, and microstructure. The focus in this talk is on how changes in alloying content, both component and concentration, affect the solidification microstructure under additive manufacturing conditions.

Non-Equilibrium Phase Transitions During Metal Additive Manufacturing

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ABSTRACT - Additive manufacturing (AM) of metal provides unique ability to produce components with complex geometries that can lead to combination of both mechanical and functional performances, that cannot be achieved by traditional manufacturing. Currently, AM technologies rely on either melting and solidification or solid-state joining of material feedstocks. The interactions between boundary conditions imposed by these processes lead to wide variations of thermal-mechanical-chemical signatures, which in turn affects the reproducibility and qualification of parts made by AM. Interestingly, this challenge is quite similar to welding and joining of metals experienced by materials and manufacturing community. In this talk, validity of extending the welding metallurgy principles to AM will be discussed with examples to demonstrate scientific solutions for minimization of defects and cracking, control of site-specific crystallographic texture and microstructure, and development of hybrid materials for extreme environments. Finally, some of the unresolved scientific questions will also be outlined and approaches to address the same will be discussed.

Acknowledgements and Disclaimer: This work relates to Department of Navy award N00014-18-1-2794 issued by the Office of Naval Research. The United States Government has a royalty-free license throughout the world in all copyrightable material contained herein. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the Office of Naval Research.

Advances in mesoscale characterization and modeling for large-scale additive manufacturing

T.K. Ales, P.C. Collins

ABSTRACT - New techniques are required to permit the characterization of the material state of material that has been produced using large-scale additive manufacturing. This talk will discuss some potential new techniques, especially a technique known as spatially resolved acoustic spectroscopy (SRAS), in the context of a review of an integrated research initiative into the interrelationships between processing, composition, microstructure, properties, and performance of large-scale additively manufactured Ti-6Al-4V. We are pursuing the development of this new technique, as it fills an important gap and permits the determination of crystal orientation over very large length scales (~10^4 sq. mms). We are also aware that periodic spatial variation in the microstructure presents some unique challenges when attempting to qualify parts and assess whether there are limiting defects. The details of this method will be presented, as will potential future application as an in-situ analysis technique to determine the materials state during additive manufacturing.

Controlling Microstructure Formation in Cast Iron

Amber Genau*, Subhojit Chakraborty, Elis Rivera-Martinez, Charlie Monroe
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ABSTRACT -Despite centuries of use and extensive study, the complex development of solidification microstructures in cast iron is still incompletely understood. Small changes in processing conditions and composition can mean the difference between graphite and carbide, or between graphite that forms flakes, nodules or vermicular structures. Unlike steel, which can be influenced with various heat treatments, the mechanical properties of cast iron are determined almost entirely by the microstructure that forms during the initial solidification process. Careful tailoring of the graphite morphology can provide sufficient ductility and a strength-to-weight ratio that allows cast iron to be used in a wider range of applications than ever before. To exploit these properties, it is necessary to understand exactly how processing parameters and composition influence microstructure formation, particularly graphite morphology, in order to control the process in a foundry. Processing via directional solidification in a Bridgman-type furnace allows for solidification velocity, thermal gradient, and composition to be precisely and independently controlled and their effects examined. This talk will describe the preparation and processing of such samples, with a particular focus on the effects of Si and Mn on flake graphite spacing, and nodularizing elements Ce and Mg on graphite morphology. The effect of microstructure on mechanical properties as measured by digital image correlation will also be discussed, along with the formation of graphite nodules as observed by deep etching and SEM.

ExaAM: Metal additive manufacturing process modeling at the fidelity of the microstructure

John Turner, ORNL; James Belak, LLNL; Chris Newman, LANL

Name and contact information of Presenter:
Chris Newman, cnewman@lanl.gov, 505-257-8274

ABSTRACT - The Exascale Computing Project (ECP, https://exascaleproject .org/) is a U.S. Dept. of Energy effort developing hardware, software infrastructure, and applications for computational platforms capable of performing 10^18 floating point operations per second (one "exaop"). The Exascale Additive Manufacturing Project (ExaAM) is one of the applications selected for development of models that would not be possible on even the largest of today's computational systems. In addition to ORNL, partners include Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), the National Institute for Standards and Technology (NIST), as well as key universities. ExaAM is leveraging existing simulation software and developing new capabilities, and we will describe the physics components that comprise our simulation environment and report on progress using highly-resolved melt pool simulations coupled in a nonlinearly consistent fashion to thermomechanics and cellular automata to drive microstructure evolution. Resulting microstructures are used to determine constitutive mechanical property relationships using polycrystal plasticity.

Los Alamos National Laboratory Agenda

5. Final Agenda (Updated 8/5/19)

MESOSCALE SCIENCE AT EXTREME CONDITIONS

Los Alamos National Laboratory and La Posada Hotel
Santa Fe, NM
August 5-9, 2019

MONDAY, AUGUST 5, 2019 – ON-SITE – LOS ALAMOS NATIONAL LABORATORY – OPEN TO Q CLEARNED BADGEHOLDERS ONLY

8:00 AM – 3:30 pm	*CLOSED SESSIONS, NISC AUDITORIUM (TA-3, Bldg. 2322)*	
8:00 – 8:30 am	Dynamic Mesoscale Materials Opportunities and Challenges (U)	John Sarrao, DDSTE
8:30 – 9:30 am	Mesoscale Applications for Integrated Experiments (U)	Grant Bazan, XTD-PRI
9:30 – 10:00 am	Material Dynamics for Secondaries (U)	John Scott, XTD-IDA
10:00 – 10:30 am	How Mesoscale Features in Explosives are Leading to Major Advancements in the Future Stockpile (U)	Von Whitley, XTD-SS
10:30 – 10:45	*Break*	
10:45 – 11:15 am	Uranium and Plutonium Casting: How Mesoscale Modeling Will Help (U)	Deniece Korzekwa, Sigma DO
11:15 – 11:45	Probing Hydrogen-Materials Interactions at the Mesoscale with X-Ray and Photon Techniques (U)	Samantha Lawrence, Sigma-2
11:45 – 12:15	Dynamic Materials Science at X-ray Light Sources: Highlights from LANL (U)	Dana Dattelbaum, M-DO
12:15 – 1:30 pm	*Lunch (On own)*	*All*
1:30 – 2:00	Plutonium Corrosion and Surface Science Opportunities for Mesoscale Research (U)	Scott Richmond, MST-16
2:00 – 2:30	Mesoscale Modeling Initiatives within ASC-PEM at LANL (U)	Marianne Francois, ALDX
2:30 – 3:00	Advanced Material Modeling in LANL's Ristra Next Generation Code Project (U)	Aimee Hungerford, XCP-DO
3:00 – 3:30	Closing Remarks and Adjourn	Abigail Hunter, XCP-5

Purpose:	Conference	Dress: Business Casual
Institutional and Technical Host:	Abigail Hunter, XCP-5 Chair, Office: 505-606-0765; Cell: 505-500-7859	
Point of Contact:	Lucy Maestas, Office: 505-667-0055; Cell: 505-699-1630	
Protocol Meeting Planner	Karen Martinez, Office: 505-665-1770; Cell: 505-231-8011	

MESOSCALE SCIENCE AT EXTREME CONDITIONS
Los Alamos National Laboratory and La Posada Hotel
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TUESDAY, AUGUST 6, 2019 – CANYON AND MONTANA BALLROOMS– LA POSADA HOTEL

7:30 – 8:00 am	*Registration and Coffee*	
8:00 – 8:30 am	Dynamic Mesoscale Materials Opportunities and Challenges	John Sarrao, DDSTE
	Session 1: Metals	
	Symposium A: Defective Metals	
8:30 – 9:00 am	The Role of Elastic and Plastic Anisotropy in Ductile Damage Nucleation along Grain Boundaries	Justin Wilkerson, Texas A&M University
9:00– 9:30 am	Non-Destructively Probing Mesoscale Radiation-Induced Microstructural Evolution	Michael Short, Massachusetts Institute of Technology
9:30 – 10:00 am	Plasticity and Fracture in Transition Metal Carbides	Giacomo Po, University of Miami
10:00 – 10:30	*Break*	
	Session 1: Metals (continued)	
	Symposium B: Multiple Principal Element/High Entropy Alloys	
10:30 – 11:00 am	Metastable High Entropy Alloys in Extreme Environments	C. Cem Tasan, Massachusetts Institute of Technology
11:00 – 11:30 am	Dislocation Dynamics in Body Centered Cubic Multi-Principal Element Alloys	Irene Beyerlein, University of California, Santa Barbara
11:30 – 12:00	Multi-principal Element Alloys for Performance in Extreme Environments	Amy Clarke, Colorado School of Mines
12:00 – 2:00 pm	*Lunch and Networking (On own)*	*All*
2:00 – 2:30	Metastability Driven Hierarchical Microstructural Engineering of Complex Concentrated Alloys for Extreme Conditions	Rajiv Mishra, University of North Texas
	Session 1: Metals (continued)	
	Symposium C: Phase Transformations	
2:30– 3:00	Modeling the Thermal and Mechanical Stability of Metastable Omega Zr”	Steve Niezgoda, Ohio State University
3:00 – 3:30	*Break*	
3:30 – 4:00	Probing Phase Transformations and Twinning Across Length Scales Using 3-D X-Ray Microscopy Techniques	Ashley Bucsek, University of Michigan
4:00 – 4:30	Proton Radiography for Dense, Dynamic Systems: A Capabilities Overview	Matthew Freeman, LANL
4:30 – 6:30	Welcome Reception and Poster Session	

MESOSCALE SCIENCE AT EXTREME CONDITIONS
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WEDNESDAY, AUGUST 7, 2019 – CANYON AND MONTANA BALLROOMS– LA POSADA HOTEL

8:00 – 8:30 am	*Registration and Coffee*	
8:30 – 10:00 am	**Session 2: High Explosives**	
8:30 – 9:00 am	Tandem Molecular Dynamics and Continuum Studies of Shock-Induced Pore Collapse in TATB	Tommy Sewell, University of Missouri
9:00 – 9:30 am	Scimitar3d: A Framework of Multiscale Simulations of Energetic Material Performance	H. S. Udaykumar, University of Iowa
9:30 – 10:00 am	The SURF Approach to Scale-Bridging: Linking Fundamental Processes to Continuum Response	Lee Perry, LANL
10:00 – 10:30	*Break*	
	Session 2: High Explosives (continued)	
10:30 – 11:00 am	Real-time Visualization of Meso-Scale Damage Evolution in Energetic Materials Under Impact	Weinong Chen, Purdue University
11:00 – 11:30 am	Mesoscale Informed Ignition and Burn Models for Weak Shock Initiation of Porous HE	Keith Gonthier, Louisiana State University
11:30 – 12:00	Interface Level Stress Measurements for Describing HE Material Mesoscale Response under Impact Loading	Vikas Tomar, Purdue University
12:00 – 2:00 pm	*Lunch and Networking (On own)*	*All*
	Session 2: High Explosives (continued)	
2:00 – 2:30	A Mesoscale Model for Shock Loading of PBX including Anisotropic Plasticity, Fracture, and Heat Transfer	Marisol Koslowski, Purdue University
2:30 – 3:00	Mesoscale Mechanics of Energetic Materials: A Coordinated Experiment-Theory Effort Using New In Situ Probes	Kyle Ramos, and Marc Cawkwell, LANL
3:00 – 3:30	*Break*	
	Session 3: Surface Science	
3:30 – 4:00	Peridynamic Models for Corrosion Damage: The Role of the Embrittled Layer in Stress Corrosion Cracking	Florin Bobaru, University of Nebraska, Lincoln
4:00 – 5:00	Wrap-up / Summarize Discussions	Abby Hunter, LANL

MESOSCALE SCIENCE AT EXTREME CONDITIONS

Los Alamos National Laboratory and La Posada Hotel

Santa Fe, NM

August 5-9, 2019

THURSDAY, AUGUST 8, 2019 – CANYON AND MONTANA BALLROOMS– LA POSADA HOTEL

8:00 – 8:30 am	*Registration and Coffee*	
8:30 – 10:00 am	**Session 4: Manufacturing**	
8:30 – 9:00 am	Modeling the Effects of Alloying on Microstructure Formation under Additive Manufacturing Conditions	Richard LeSar, Iowa State University
9:00 – 9:30 am	Non-Equilibrium Phase Transitions During Metal Additive Manufacturing	Suresh Babu, University of Tennessee, Knoxville
9:30 – 10:00 am	Advances in Mesoscale Characterization and Modeling for Large-Scale Additive Manufacturing	Peter Collins, Iowa State University
10:00 – 10:30	*Break*	
	Session 4: Manufacturing (continued)	
10:30 – 11:00 am	Controlling Microstructure Formation in Cast Iron	Amber Genau, University of Alabama
11:00 – 11:30 am	ExaAM: Metal Additive Manufacturing Process Modeling at the Fidelity of the Microstructure	Christopher Newman, LANL
11:30 – 12:00	Summary of Workshop and Closing Remarks	Abigail Hunter, LANL
12:00 – 2:00 pm	*Adjourn*	